LOSS OF CHAOTICITY DURING β-TURN TRANSITION: DYNAMIC COMPLEXITY OF PROTEIN FOLDING

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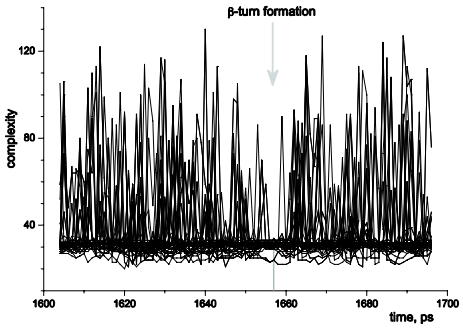
ABSTRACT

An elementary event of protein folding - the β-turn formation - in a Leu-enkephalin molecule is investigated. Classical MD of the peptide in explicit water is used to simulate the trajectories of the system's atoms. They are then analysed using the computational mechanics[1] approach in order to discover the dynamic structure at the moment of turn formation. It is found that all the peptide's atoms as well as the majority of the waters of the first solvation shell exhibit a drop in dynamic complexity exactly at the moment of the transition. The complexity measure used in this study quantify the degree of chaoticity of the system's trajectories, the more chaotic corresponding to a higher value of complexity. Transition dynamics theory suggests that chaotic dynamics can become quasi-regular at the moment of barrier crossing[2]. Thus our results present the first evidence supporting this general hypothesis for realistic high-dimensional molecular systems.



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[1] J.P. Crutchfield, D.P. Feldman, and C.R. Shalizi, *Phys. Rev. E*, **2000**, *62*, 2996.

[2] T. Komatsuzaki and R.S. Berry, *Adv. Chem. Phys.*, **2002**, *123*, 79.